

Stochastic Methods for Quantum Scattering

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ABSTRACT

Quantum scattering at zero energy is studied with stochastic methods. A path integral representation for the scattering cross section is developed. It is demonstrated that Monte Carlo simulation can be used to compare effective potentials which are frequently used in multiple scattering with the exact result.

1. Introduction

Multiple scattering off nuclei is in general a complicated many body problem, as target and projectile degrees of freedom are strongly coupled. The standard method for treating multiple scattering problems is the construction of an effective one-body optical model potential by eliminating the target degrees of freedom. Optical potential calculations have been widely and very successfully used in the past [1].

Despite their phenomenological success, there are severe shortcomings of these models. One example is the spectrum of kaonic atoms, where the shifts of the lowest level require a repulsive real part of the optical potential, in contrast to the results of conventional fits [2]. Another problem, which is conceptually even more severe, is the absence of reliable methods for calculating inclusive cross sections, for which optical potential models can not be applied at all, as they are based on restriction of the target Hilbert space.

Because of these problems, alternative methods have to be studied. For calculating ground state properties of a many body system beyond perturbative or mean field approximations, stochastic methods are well established. Starting from a path integral expression for the density matrix, an algorithm of Metropolis type or Langevin simulation is used for path sampling [3]. The advantage of these approaches is that they provide results, which are in principle exact and can be used to develop better analytical understanding of the physical system under investigation.

2. Path integrals and scattering observables

We start from a Hamiltonian

$$H = H_{int} + \frac{p^2}{2m} + V$$

which can be decomposed into an internal target Hamiltonian H_{int} , a projectile kinetic energy and a projectile-target interaction V . In case the projectile has no bound state, the ground state of the system is the zero projectile momentum scattering wave function $\Psi_{0,k=0}(x, q)$. In the low temperature limit, the density matrix of the system is dominated by this state [4]:

$$\rho(x'q, xq|\beta) = \langle x'q' | e^{-\beta H} | xq \rangle \stackrel{\beta \rightarrow \infty}{=} e^{-\beta E_0} \left(\frac{2\pi m}{\beta} \right)^{3/2} \Psi_{0,k=0}(x', q') \Psi_{0,k=0}^\dagger(x, q) \quad (1)$$

q denotes the target and x the projectile degrees of freedom. E_0 is the target ground state energy. In pure bound state problems, convergence is controlled by the energy gap between first excited state and ground state. Here, the ground state of the system lies at the edge of a continuum. This fact manifests itself in the $\beta^{3/2}$ factor in front of eq.(1). The slow convergence, as compared with bound state problems, requires rather long times β , which makes it necessary to choose observables and path sampling techniques carefully.

From the left hand side of (1), a path integral expression can be derived [5] in the standard way. Path sampling methods, however, do not yield the path integral directly, but give only paths sampled according to the normalized functional

$$P[x(t), q(t)] := \frac{\exp(-S[x(t), q(t)])}{\int d[x]d[q] \exp(-S[x(t), q(t)])}. \quad (2)$$

This difficulty can be solved by measuring the following functional:

$$O[x(t), q(t)] = \exp \int dt [V(x(t), q(t)) - U(x(t))] \quad (3)$$

The interaction between projectile and target is removed from the numerator and replaced by an effective interaction U , which only acts on the projectile degrees of freedom, like in conventional treatment of multiple scattering physics. The advantage here is, that the stochastic process can be used to test the quality of the effective potential U . The expectation value of O in P is in the limit $\beta \rightarrow \infty$:

$$\langle O \rangle \stackrel{\beta \rightarrow \infty}{=} \frac{\Phi_0(q)\Phi_0(q')\psi_{k=0}(x')\psi_{k=0}^\dagger(x)}{\Psi_{0,k=0}(x'q')\Psi_{0,k=0}^\dagger(xq)},$$

where Φ_0 is the target ground state and $\psi_{k=0}$ is the projectile scattering wave function to the potential U .

3. Example: Potential Scattering

To demonstrate the feasibility of this type of calculations I discuss potential scattering. In this case numerical integration of the Schroedinger equation provides exact results. Scattering off a Gaussian potential V_g is considered. As reference potential a square well V_w is used:

$$V_g(r) = V_0 \exp(-\frac{1}{2}r^2) \quad V_w(r) = \begin{cases} 3\sqrt{\frac{\pi}{250}}V_0 & , r < \sqrt{5} \\ 0 & , r > \sqrt{5} \end{cases}$$

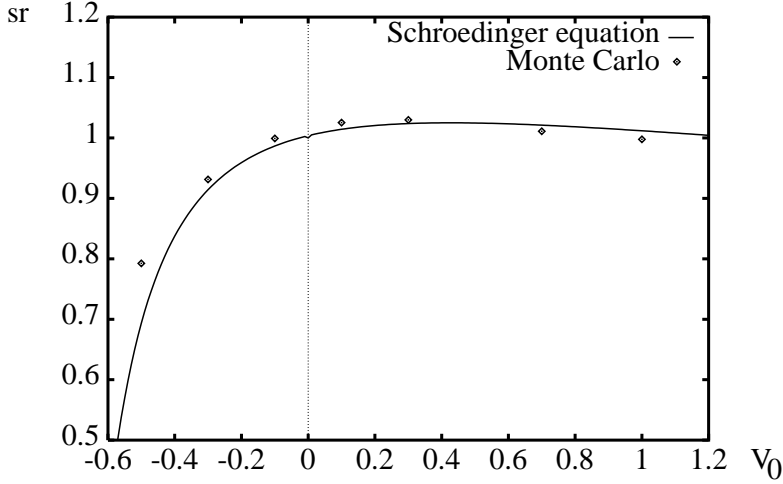


Figure 1: Ratio of cross sections of square well potential and Gaussian potential sr as function of potential strength V_0 . The line is the exact result, the data points are a stochastic calculation at $\beta = 100$. The path was subdivided into 200 time intervals $\Delta\beta = 0.5$. The projectile mass was set to $m = 1$.

V_w plays the role of the effective potential U in (3). The parameters of the square well are fitted to reproduce the first two nonvanishing moments of the Gaussian potential. Fig.1 shows the ratio of the cross sections of the two potentials $sr := \sigma_{V_w}/\sigma_{V_g}$ as a function of V_0 . The line is the exact result, the data points are obtained from a stochastic calculation at $\beta = 100$. Path sampling was performed with a simple forward Euler scheme Langevin algorithm [6]. 2.5×10^5 paths were used to measure O after an equilibration run of 2.5×10^4 updates.

In the range of V_0 where the reference potential is already a good guess, the stochastic calculation reproduces the exact result within 2%. Where this is no longer true, results become worse. For $V_0 = -0.5$ the stochastic result deviates about 17%. Note that at this value of V_0 the cross section is already $\sigma = 274$, because V_g has the first bound state at $V_0 = -0.66$. There are two ways to improve the results in this region: One possibility is to increase β . This would require much longer calculation times, as the autocorrelation time of the Langevin algorithm increases like β^2 . The other possibility is to improve the reference potential. By adjusting the parameters of the potential successively, one can obtain results for the stochastic calculation which do not deviate more than a few percent from the exact result, although the same simulation parameters as for the first calculation were used.

4. Discussion

A new method for calculating elastic cross sections at zero projectile momentum was

presented. The crucial point is that this method relies on the comparison of the full problem with a reference problem. This makes it possible to study questions related to the construction of effective potentials in nuclear multiple scattering by computer simulations, which seems to be the natural way for a nonperturbative treatment of many body problems. The method can be extended to nonzero momentum by exploiting information contained in the β dependence of observables. Work in this direction, as well as multiple scattering calculations, are currently in progress.

A severe shortcoming of this method is that at this stage it is not possible to calculate inelastic or inclusive cross sections. Developement of stochastic methods for these problems seems to be promising, as scattering observables will not depend strongly on individual nuclear states due to summation over final states. The simple structure of experimental data like e.g. energy loss spectra [1] strongly supports this conjecture.

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